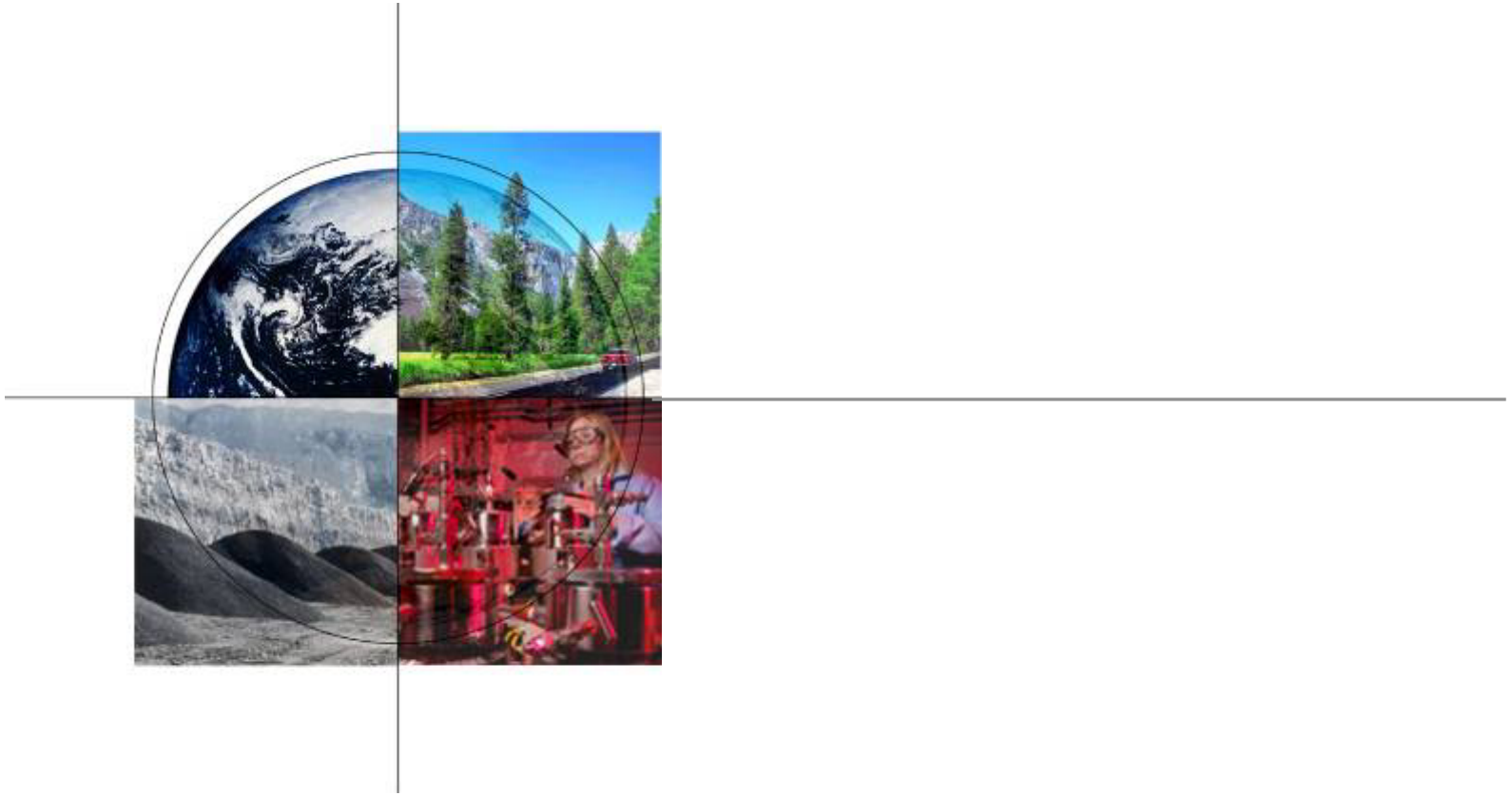
Modeling for the rapid development of advanced carbon management technologies



National Energy Technology Laboratory

Office of Fossil Energy

Carbon Management

- **Reducing the Carbon Footprint**
  - Higher Efficiency
  - Biomass/Coal Gasification and Fuels Production
- **Carbon Capture and Separation**
  - Conventional
  - Unconventional
- **Carbon Storage**
  - Storage Opportunities
  - Interaction with regional partnerships
  - Measurement, monitoring, and verification
- **Risk Assessment**
  - Long-term reactivity
  - Modeling long term behavior
  - Incorporation of other systems analysis

CCS Modeling at NETL

Capture Modeling

Plant
- IECM
- Aspen Plus
- APECS

Device
MFIX
FLUENT

Atomic Scale
VASP
accelrys suite
GAUSSIAN

Sequestration Modeling

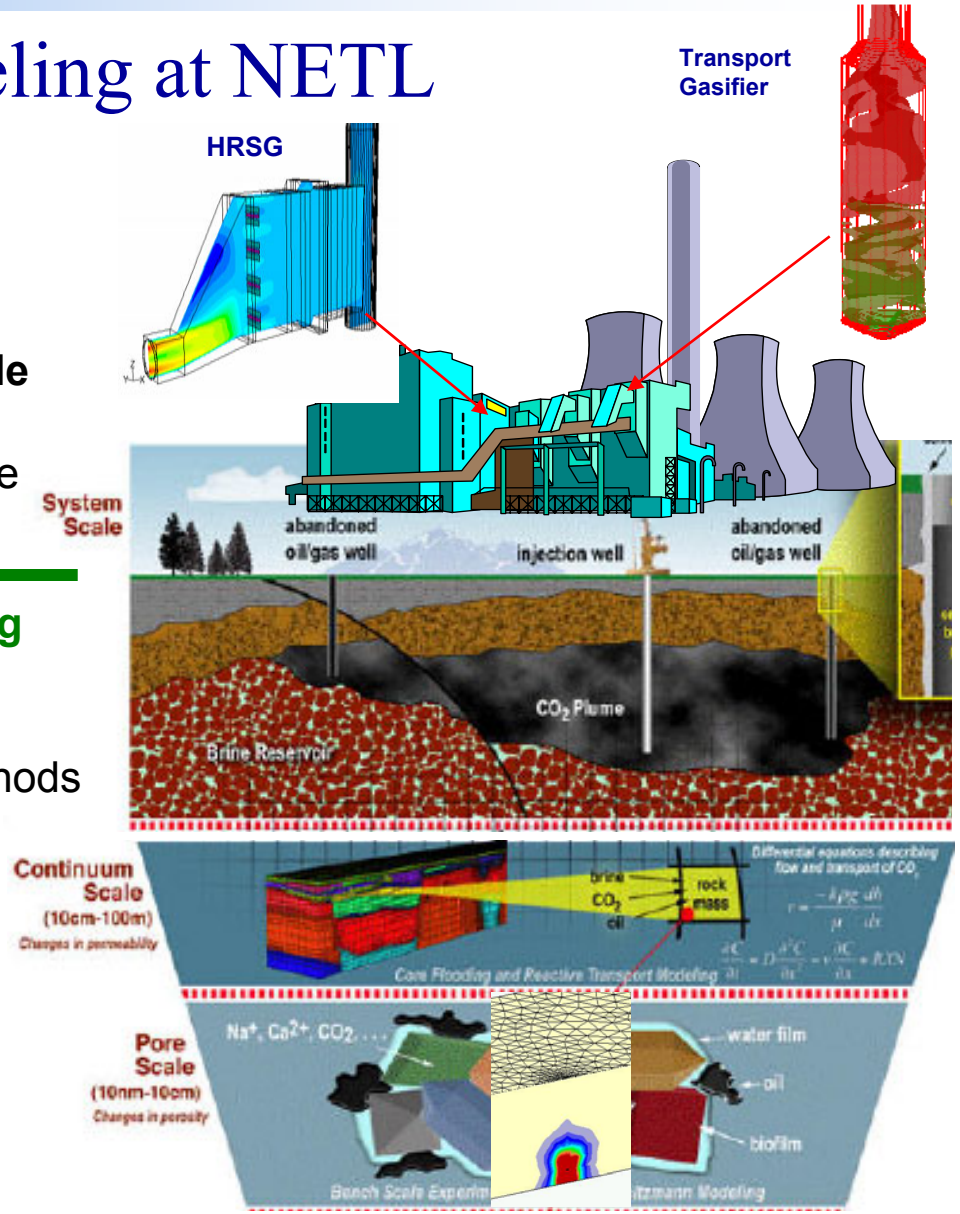
Reservoir/coal bed
PSU-COALCOMP
NFFLOW

Continuum/Pore scale
FLUENT
NETFlow

Geomechanics
SEQURE
ABAQUS

MMV Modeling

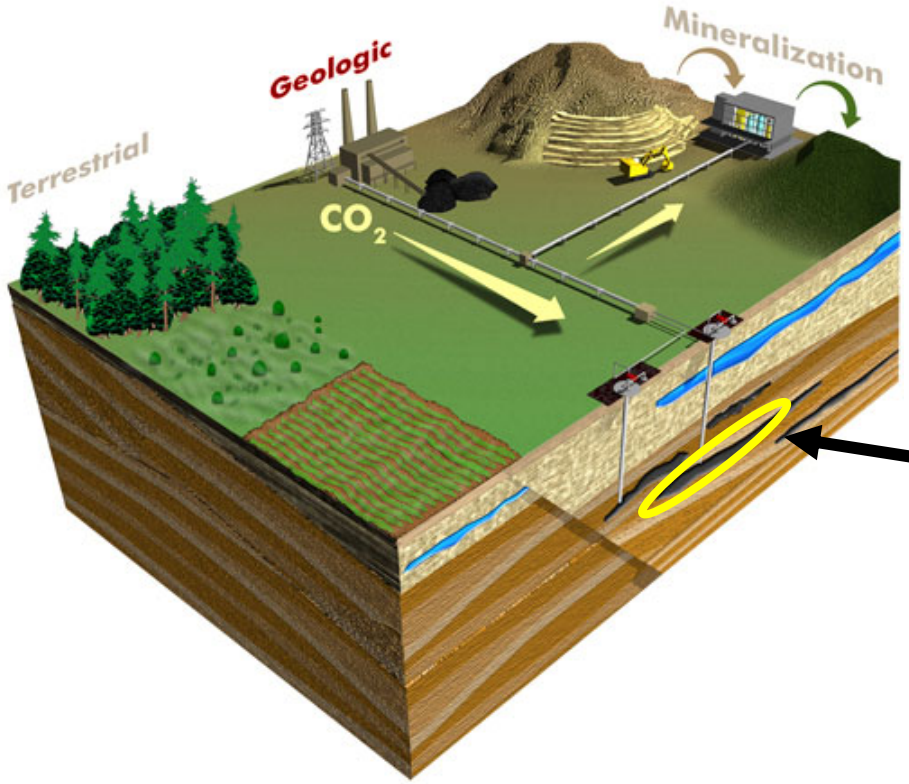
NFFLOW
TOUGH2
Statistical methods



Summary of Simulation Work for Geologic Sequestration and Related Research

- Development of simulation capabilities for the injection CO_2 into coal seams, particularly related to coal swelling
- Pore-level simulations help understand fundamentals of two-phase flow, scaling laws, and capacity predictions
- Fracture flow simulations help understand fundamentals of two-phase fracture flow and better model CO_2 sequestration in non-traditional reservoirs, as well as migration through faults and fracture networks
- Geomechanical and flow modeling identifies subsurface regions where additional rock stresses form, as well as help predict sequestration capacities
- Flow modeling and statistical techniques help design monitoring networks and interpret data from them

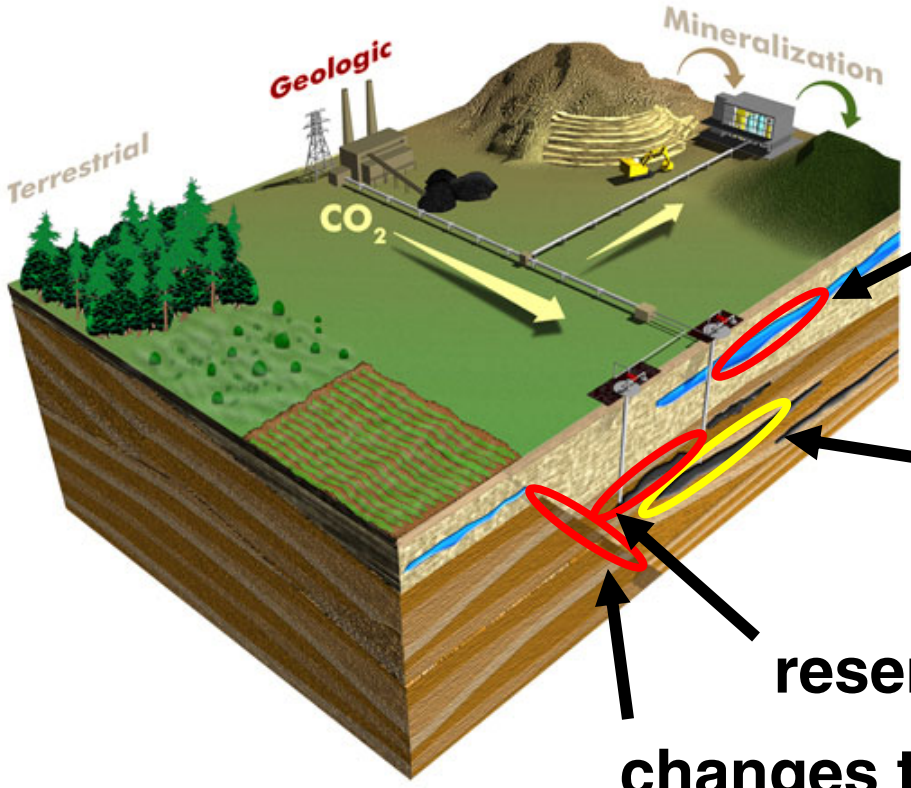
Quantitative risk assessment is a formal process to minimize potential consequences of long-term storage.



CO_2 storage reservoir

Risk assessment must consider the potential for CO_2 release and subsequent movement from storage reservoir to various receptors.

Goal is to minimize the potential impact to subsurface receptors.



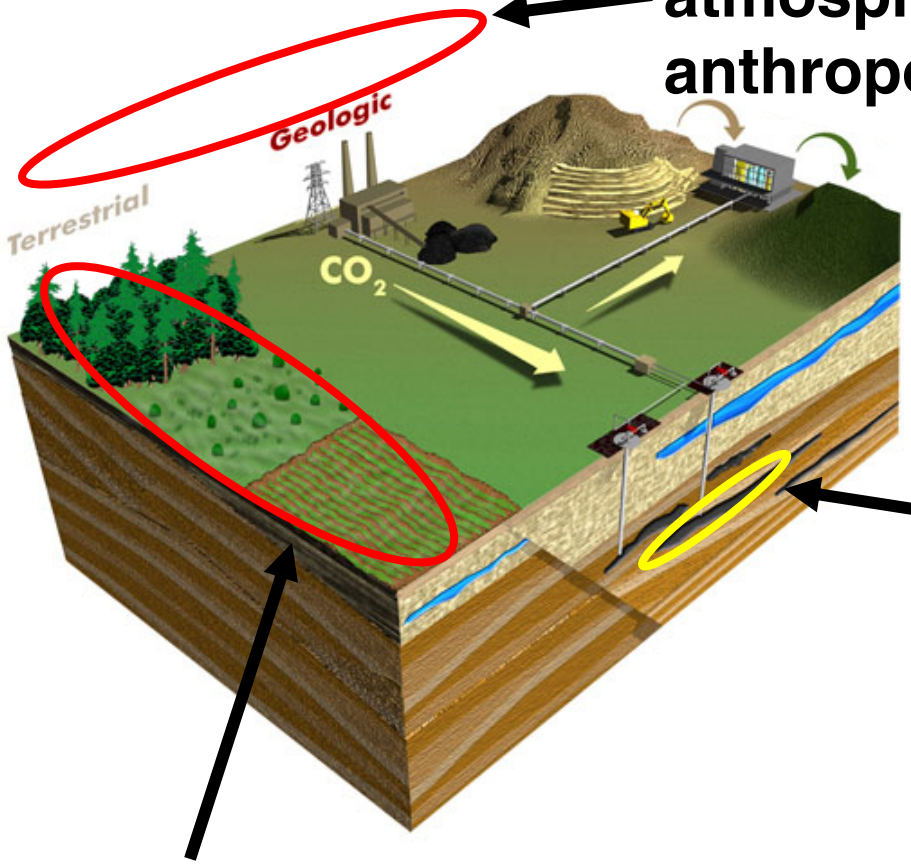
groundwater

CO_2 storage reservoir

reservoirs for other resources

changes to faults

Goal is to minimize the potential impact to surface receptors.

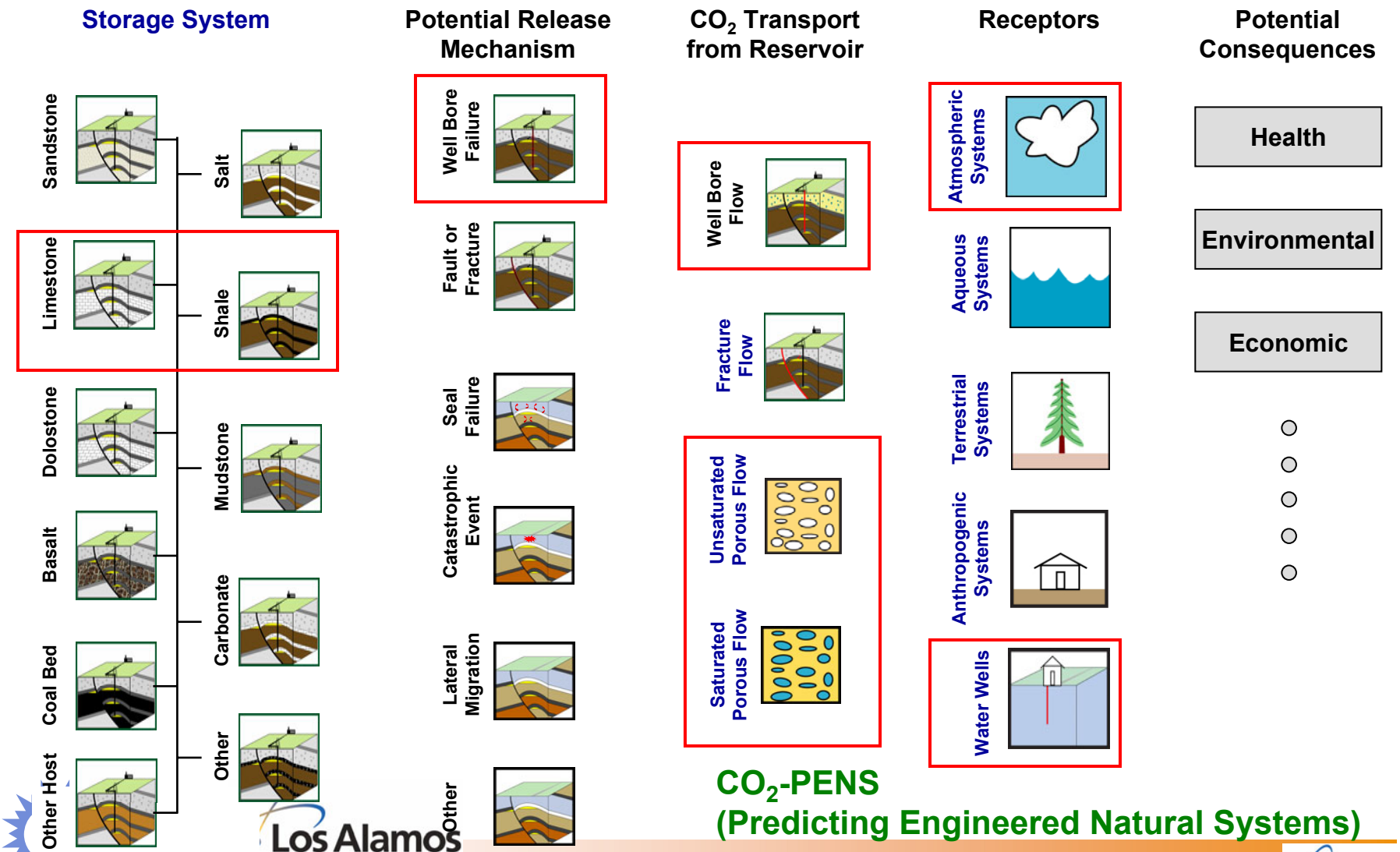


atmosphere;
anthropogenic systems

CO_2 storage reservoir

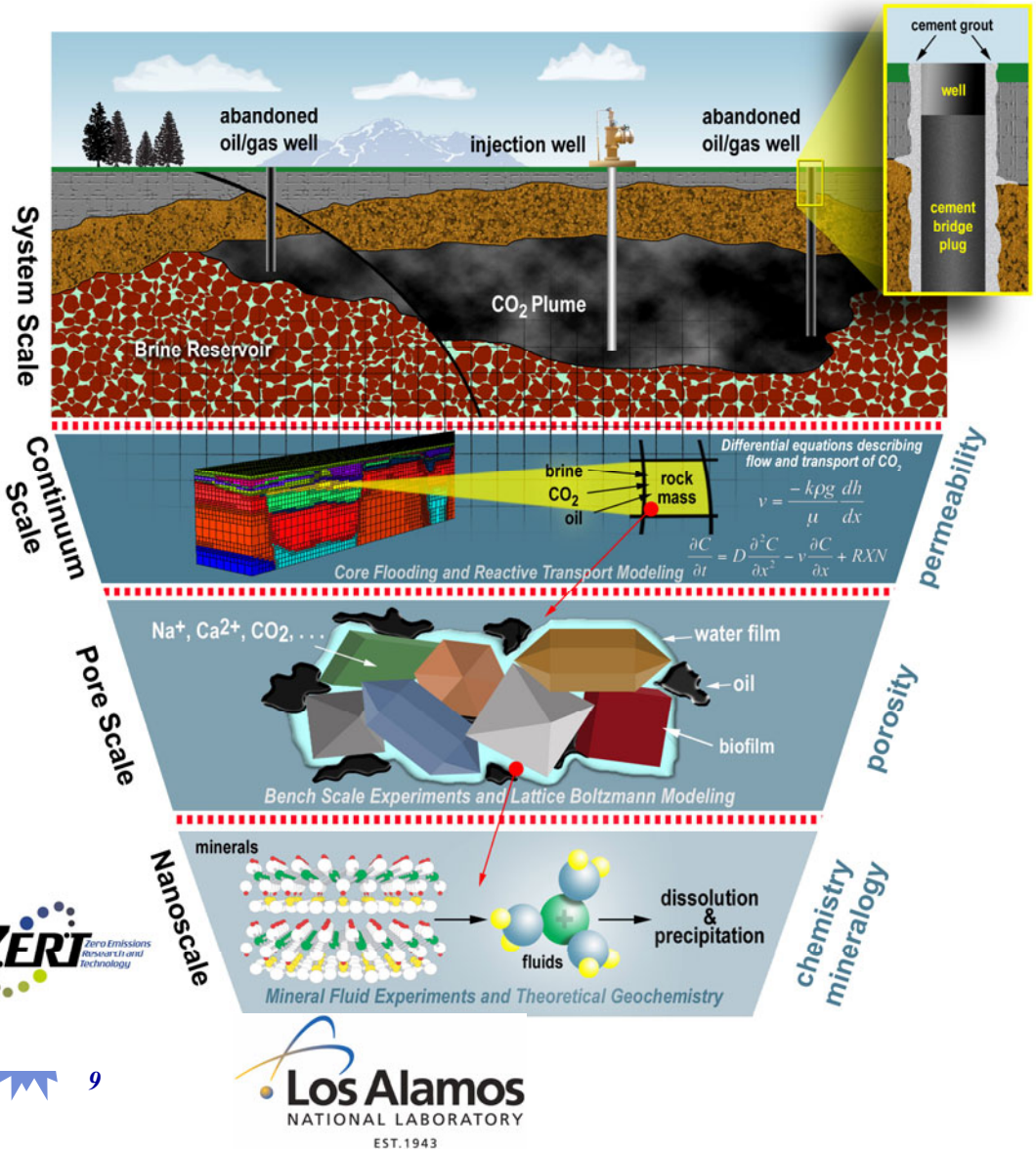
terrestrial ecosystems; subaqueous systems

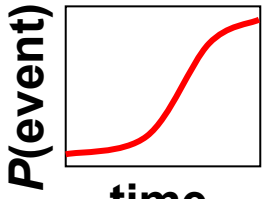
CO_2-PENS Risk Assessment Framework



CO_2-PENS
(Predicting Engineered Natural Systems)

Science based prediction of natural system performance requires system-level probabilities based on process level phenomena.





ry,
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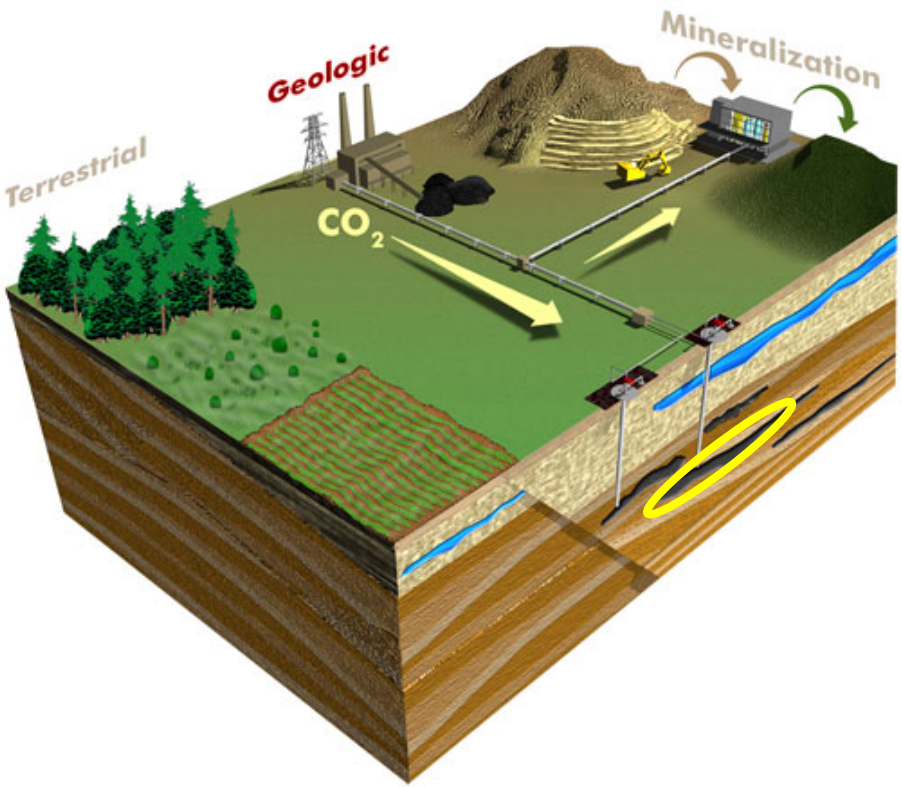
observation (analog sites)

Storage Reservoir Factors to Consider in Risk Assessment



Key Features/Events/Processes

- geologic characteristics
  - porosity/permeability
  - lithologic unit(s) (chemistry; mineralogy)
  - geologic structure
  - heterogeneity
  - existing fluids (brine; oil/gas)
- containment characteristics
  - vertical seal(s); horizontal seal(s)
  - storage-unit volume
- long-term reactions
  - dissolution into brine (reverses buoyancy)
  - reaction with reservoir rock (mineralizes)

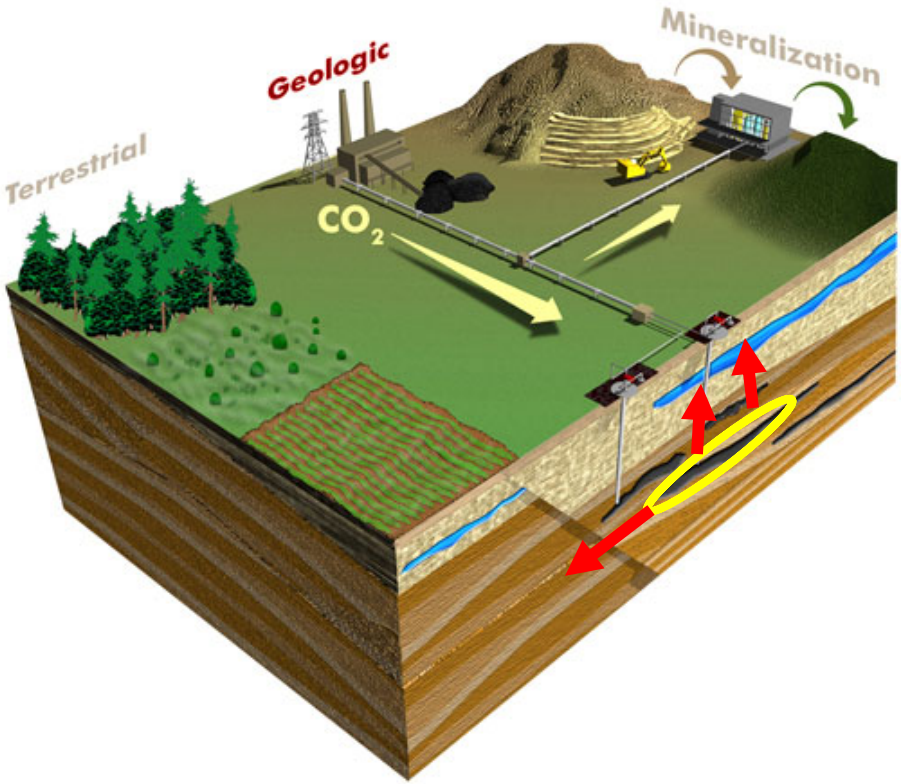
Factors to Consider

- Injection wells needed; existing injection/water wells
- Displacement of reservoir fluids
- Change in physical conditions
- Insufficient capacity

Current CO_2-PENS Approach

- GIS tool can extract site-specific information from databases (e.g., wellbores, reservoirs, etc.)
- continuum-scale reactive transport DLL
- simplified analytical model for growth of plume and pressure field

Potential Release and Transport Mechanisms to Consider



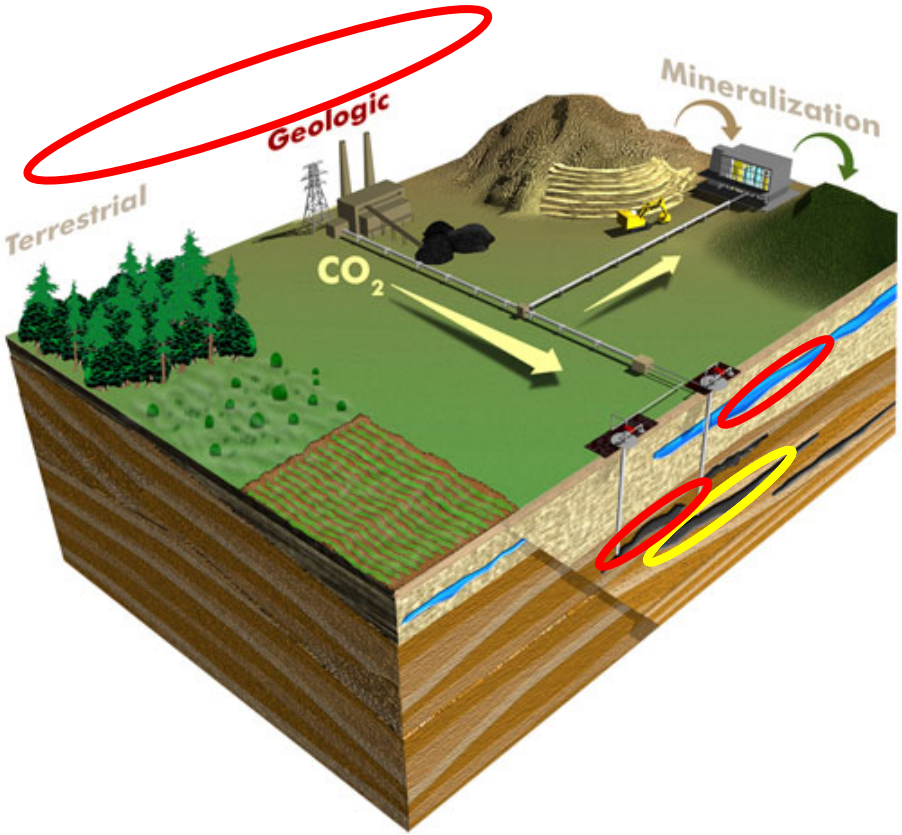
Key Features/Events/Processes

- wellbore release
  - poor (no) completion
  - corrosion of cement or casing
- release through seal
  - fractures/faults; diffusion
- lateral migration
- fastpath transport (including wellbores)
- porous flow (saturated and unsaturated)

Current CO_2-PENS Approach

- Princeton wellbore model for release/transport
- simple diffusion through seal
- simple capacity overflow for lateral migration
- continuum-scale transport out of reservoir under development

Potential Receptor Impacts to Consider



Key Features/Events/Processes

- resource-reservoir impacts
  - CO_2 migrates to another reservoir (oil, gas, pore space, etc.)
- groundwater impacts
  - CO_2 accumulation followed by water-rock interactions and transport
- atmospheric impacts
  - CO_2 return to the atmosphere
  - mixing in atmosphere affects CO_2 level

Current CO_2-PENS Approach

- tracks CO_2 accumulation and migration from wellbore release (Princeton analytical model)
- couples USGS water-rock model (PHREEQ)
- allows boundary-layer mixing in simple analytical solution with local metereological conditions drawn from database

Virtual Power Plant with Carbon Management